



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 02:06 AM EDT

PDB ID : 5KQ3 / pdb_00005kq3
Title : Crystal structure of the D141A/Q233E variant of catalase-peroxidase from *B. pseudomallei*
Authors : Loewen, P.C.
Deposited on : 2016-07-05
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

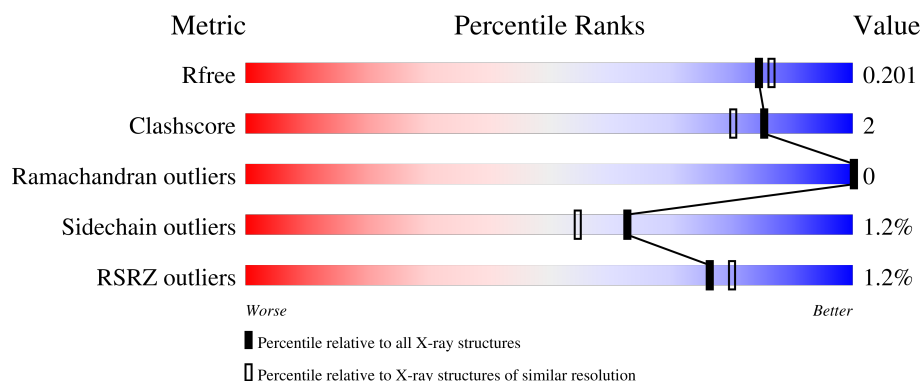
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	% 90% 7% ..
1	B	728	% 90% 7% ..

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12481 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

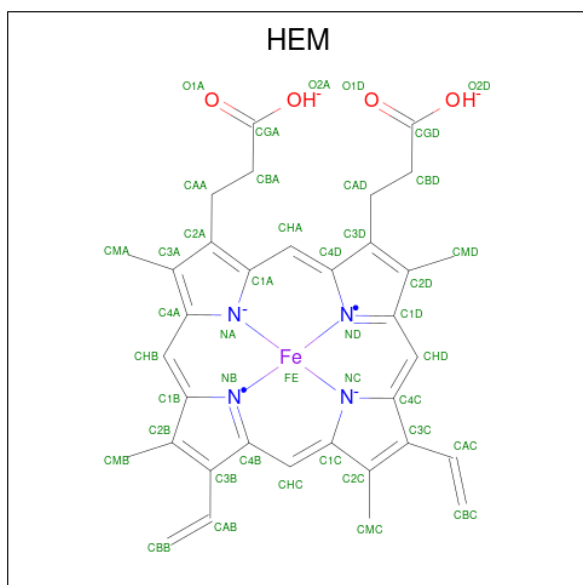
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	7	0
			5553	3505	990	1044	14			
1	B	713	Total	C	N	O	S	0	6	0
			5537	3497	984	1042	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	engineered mutation	UNP Q3JNW6
A	233	GLU	GLN	engineered mutation	UNP Q3JNW6
B	141	ALA	ASP	engineered mutation	UNP Q3JNW6
B	233	GLU	GLN	engineered mutation	UNP Q3JNW6

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

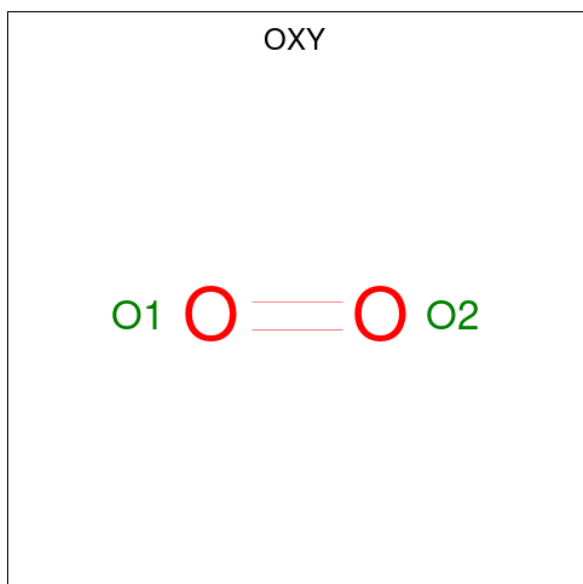
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



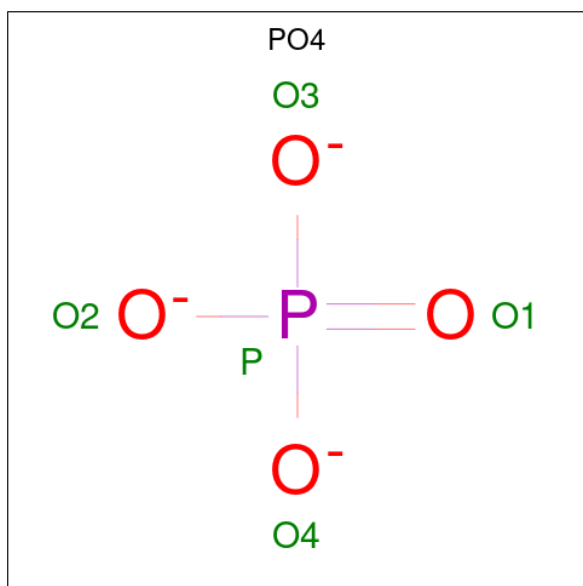
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		

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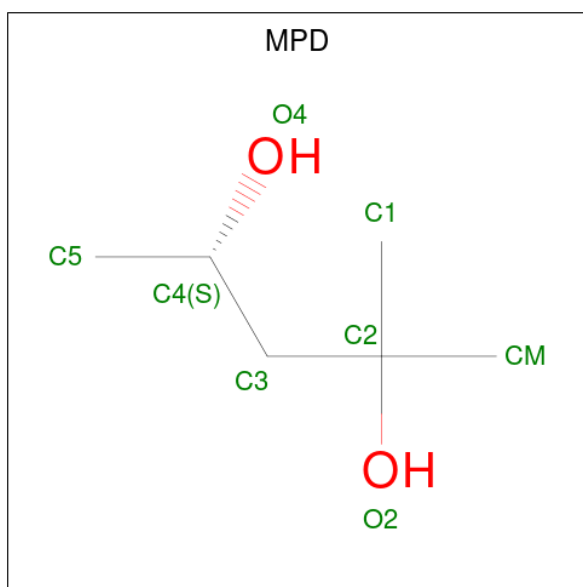
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			2	2		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		

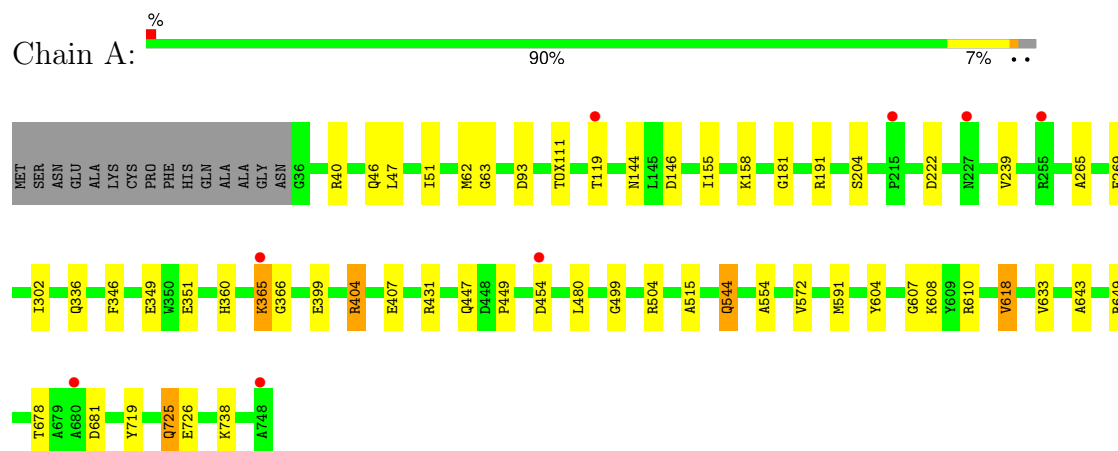
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	622	Total	O	0	0
			622	622		
8	B	633	Total	O	0	0
			633	633		

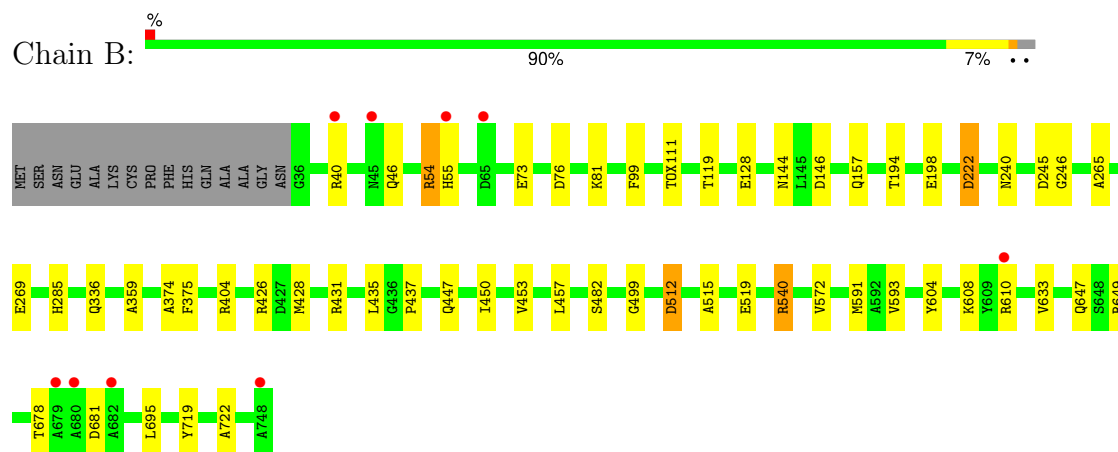
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Catalase-peroxidase



• Molecule 1: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.04Å 114.03Å 174.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.73 – 1.85 47.73 – 1.85	Depositor EDS
% Data completeness (in resolution range)	88.8 (47.73-1.85) 88.9 (47.73-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.159 , 0.195 0.170 , 0.201	Depositor DCC
R_{free} test set	7578 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12481	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OXY, CL, TOX, NA, PO4, HEM, MPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.45	22/5681 (0.4%)	1.14	6/7720 (0.1%)
1	B	1.45	17/5668 (0.3%)	1.15	5/7704 (0.1%)
All	All	1.45	39/11349 (0.3%)	1.14	11/15424 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	512	ASP	CG-OD2	7.48	1.39	1.25
1	A	349	GLU	C-O	-7.45	1.15	1.23
1	A	499	GLY	C-O	7.03	1.30	1.23
1	B	437	PRO	C-O	-6.84	1.15	1.24
1	A	222	ASP	CA-C	6.31	1.60	1.53
1	A	204	SER	N-CA	6.10	1.54	1.46
1	A	618	VAL	CA-C	5.95	1.60	1.52
1	B	375	PHE	CA-CB	-5.91	1.43	1.53
1	A	643	ALA	C-O	-5.90	1.16	1.24
1	B	450	ILE	C-O	-5.89	1.17	1.24
1	A	544	GLN	CD-OE1	5.86	1.34	1.23
1	A	725	GLN	CG-CD	5.81	1.66	1.52
1	A	607	GLY	N-CA	5.79	1.50	1.45
1	B	285	HIS	N-CA	5.77	1.53	1.46
1	B	222	ASP	CA-C	5.70	1.59	1.53
1	B	482	SER	CA-CB	5.67	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLY	N-CA	5.61	1.52	1.45
1	A	346	PHE	CA-C	5.50	1.59	1.52
1	B	285	HIS	C-O	5.48	1.30	1.24
1	A	155	ILE	CA-C	5.47	1.59	1.52
1	A	365	LYS	N-CA	5.43	1.53	1.46
1	B	722	ALA	C-O	-5.36	1.17	1.24
1	A	191	ARG	CA-C	5.35	1.59	1.52
1	A	399	GLU	C-O	-5.34	1.17	1.24
1	A	572	VAL	C-O	-5.33	1.17	1.24
1	B	499	GLY	C-O	5.30	1.29	1.24
1	B	572	VAL	C-O	-5.28	1.17	1.24
1	A	504	ARG	N-CA	-5.28	1.39	1.46
1	A	158	LYS	C-O	-5.25	1.18	1.24
1	B	359	ALA	CA-C	-5.24	1.46	1.52
1	B	426	ARG	CZ-NH2	5.20	1.40	1.33
1	B	240	ASN	CA-C	5.18	1.58	1.52
1	B	245	ASP	CA-CB	5.17	1.61	1.53
1	A	449	PRO	N-CA	-5.12	1.40	1.47
1	B	157	GLN	N-CA	-5.12	1.40	1.46
1	A	239	VAL	N-CA	5.10	1.52	1.46
1	A	407	GLU	CG-CD	5.02	1.64	1.52
1	A	404	ARG	N-CA	-5.01	1.40	1.46
1	B	194	THR	CA-C	5.00	1.58	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	591	MET	CG-SD-CE	-6.38	86.87	100.90
1	B	428	MET	CA-CB-CG	-5.69	102.71	114.10
1	A	591	MET	CG-SD-CE	-5.60	88.59	100.90
1	B	246	GLY	N-CA-C	5.34	122.73	115.30
1	A	46	GLN	N-CA-CB	5.27	117.90	110.36
1	B	46	GLN	N-CA-CB	5.21	117.81	110.36
1	A	62	MET	CA-C-N	-5.17	114.80	120.44
1	A	62	MET	C-N-CA	-5.17	114.80	120.44
1	A	93	ASP	N-CA-C	5.09	117.56	111.71
1	A	181	GLY	N-CA-C	5.07	122.58	115.43
1	B	512	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5553	0	5360	22	1
1	B	5537	0	5348	22	1
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	24	0	42	3	0
7	B	8	0	14	1	0
8	A	622	0	0	5	2
8	B	633	0	0	8	2
All	All	12481	0	10824	48	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198[A]:GLU:OE1	8:B:901:HOH:O	1.69	1.09
1:B:119[B]:THR:HG21	8:B:1097:HOH:O	1.67	0.93
1:A:119[B]:THR:HG21	8:A:1076:HOH:O	1.71	0.88
1:A:725:GLN:NE2	1:A:726[A]:GLU:HG3	2.04	0.72
7:A:807:MPD:H53	7:A:807:MPD:H11	1.72	0.71
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.28	0.68
1:B:647:GLN:HG2	8:B:932:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:O	8:A:902:HOH:O	2.13	0.66
1:B:519:GLU:OE1	8:B:902:HOH:O	2.13	0.66
1:B:76:ASP:OD2	8:B:903:HOH:O	2.13	0.66
1:B:336:GLN:HB3	8:B:1410:HOH:O	2.00	0.61
7:B:806:MPD:H53	7:B:806:MPD:HM1	1.82	0.61
1:A:351:GLU:OE2	1:A:365:LYS:HD3	2.00	0.60
1:A:351:GLU:HB2	1:A:365:LYS:CE	2.32	0.60
1:A:351:GLU:HB2	1:A:365:LYS:NZ	2.21	0.56
1:A:725:GLN:NE2	1:A:726[A]:GLU:CG	2.71	0.54
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.92	0.53
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.92	0.53
1:A:738:LYS:NZ	8:A:913:HOH:O	2.41	0.52
1:B:512:ASP:HB2	8:B:1165:HOH:O	2.10	0.51
1:B:73:GLU:OE1	1:B:435:LEU:HD22	2.12	0.50
7:A:807:MPD:H11	7:A:807:MPD:C5	2.41	0.49
1:B:540:ARG:NE	1:B:540:ARG:HA	2.28	0.49
1:A:351:GLU:HB2	1:A:365:LYS:HE2	1.95	0.48
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.16	0.46
1:B:119[B]:THR:HG23	1:B:593:VAL:HG11	1.98	0.46
1:A:269:GLU:OE1	1:A:404:ARG:NH2	2.45	0.46
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.46	0.45
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.16	0.45
1:A:360:HIS:ND1	8:A:909:HOH:O	2.36	0.45
1:A:454:ASP:OD2	1:A:454:ASP:N	2.47	0.45
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.17	0.44
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.17	0.44
1:A:480:LEU:HD22	1:A:554:ALA:HB1	1.99	0.44
1:A:515:ALA:HB2	1:A:604:TYR:CE2	2.54	0.43
1:B:678:THR:OG1	1:B:681:ASP:O	2.33	0.43
1:B:269:GLU:OE1	1:B:404:ARG:NH2	2.45	0.43
1:B:99:PHE:CD2	1:B:374:ALA:HA	2.54	0.43
1:A:119[A]:THR:HG21	1:A:265:ALA:HB2	1.99	0.43
1:B:81:LYS:NZ	8:B:927:HOH:O	2.52	0.43
1:B:515:ALA:HB2	1:B:604:TYR:CE2	2.53	0.43
1:A:678:THR:OG1	1:A:681:ASP:O	2.36	0.42
1:A:51:ILE:HD11	1:A:618:VAL:HG12	2.02	0.42
1:A:336[B]:GLN:HG3	8:A:987:HOH:O	2.19	0.41
1:B:453:VAL:HG11	1:B:457:LEU:HD21	2.03	0.41
1:B:128:GLU:OE1	1:B:198[A]:GLU:HG3	2.21	0.41
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.50	0.41
7:A:807:MPD:C5	7:A:807:MPD:C1	2.99	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1379:HOH:O	8:B:1440:HOH:O[4_445]	1.93	0.27
8:A:1426:HOH:O	8:B:1463:HOH:O[4_445]	1.93	0.27
1:A:365:LYS:NZ	1:B:695:LEU:O[3_544]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	716/728 (98%)	705 (98%)	11 (2%)	0	100	100
1	B	715/728 (98%)	706 (99%)	9 (1%)	0	100	100
All	All	1431/1456 (98%)	1411 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	554/559 (99%)	548 (99%)	6 (1%)	65	57
1	B	553/559 (99%)	546 (99%)	7 (1%)	61	51
All	All	1107/1118 (99%)	1094 (99%)	13 (1%)	63	55

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	302	ILE
1	A	544	GLN
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	54	ARG
1	B	222	ASP
1	B	540	ARG
1	B	608	LYS
1	B	610	ARG
1	B	649	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	247	ASN
1	A	725	GLN
1	B	46	GLN
1	B	406	HIS
1	B	544	GLN
1	B	725	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TOX	B	111[A]	2	14,17,18	1.72	2 (14%)	12,23,25	2.00	4 (33%)
1	TOX	A	111[B]	-	14,17,18	2.34	6 (42%)	12,23,25	3.16	6 (50%)
1	TOX	B	111[B]	-	14,17,18	1.72	2 (14%)	12,23,25	2.00	4 (33%)
1	TOX	A	111[A]	2	14,17,18	2.34	6 (42%)	12,23,25	3.16	6 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TOX	B	111[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	A	111[A]	2	-	2/5/8/10	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	O-C	5.29	1.40	1.20
1	B	111[B]	TOX	O-C	5.29	1.40	1.20
1	A	111[A]	TOX	O-C	4.41	1.36	1.20
1	A	111[B]	TOX	O-C	4.41	1.36	1.20
1	A	111[A]	TOX	CD2-CE2	3.94	1.46	1.41
1	A	111[B]	TOX	CD2-CE2	3.94	1.46	1.41
1	A	111[A]	TOX	CD1-CG	3.68	1.44	1.36
1	A	111[B]	TOX	CD1-CG	3.68	1.44	1.36
1	A	111[A]	TOX	CH2-CZ2	2.71	1.43	1.38
1	A	111[B]	TOX	CH2-CZ2	2.71	1.43	1.38
1	A	111[A]	TOX	CH2-CZ3	2.68	1.44	1.38
1	A	111[B]	TOX	CH2-CZ3	2.68	1.44	1.38
1	B	111[A]	TOX	CH2-CZ3	2.08	1.42	1.38
1	B	111[B]	TOX	CH2-CZ3	2.08	1.42	1.38
1	A	111[A]	TOX	CA-N	-2.06	1.42	1.48
1	A	111[B]	TOX	CA-N	-2.06	1.42	1.48

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CZ2-CE2-CD2	-7.15	113.97	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[B]	TOX	CZ2-CE2-CD2	-7.15	113.97	121.95
1	A	111[A]	TOX	CZ2-CE2-NE1	3.81	135.44	129.37
1	A	111[B]	TOX	CZ2-CE2-NE1	3.81	135.44	129.37
1	A	111[A]	TOX	CE2-CD2-CG	-3.69	104.00	107.39
1	A	111[B]	TOX	CE2-CD2-CG	-3.69	104.00	107.39
1	A	111[A]	TOX	CE3-CD2-CE2	3.67	123.47	119.24
1	A	111[B]	TOX	CE3-CD2-CE2	3.67	123.47	119.24
1	A	111[A]	TOX	CH2-CZ2-CE2	3.53	125.40	118.28
1	A	111[B]	TOX	CH2-CZ2-CE2	3.53	125.40	118.28
1	B	111[A]	TOX	CZ2-CE2-NE1	3.46	134.89	129.37
1	B	111[B]	TOX	CZ2-CE2-NE1	3.46	134.89	129.37
1	A	111[A]	TOX	CZ3-CH2-CZ2	-3.26	116.21	120.24
1	A	111[B]	TOX	CZ3-CH2-CZ2	-3.26	116.21	120.24
1	B	111[A]	TOX	CZ3-CH2-CZ2	-3.25	116.23	120.24
1	B	111[B]	TOX	CZ3-CH2-CZ2	-3.25	116.23	120.24
1	B	111[A]	TOX	CZ2-CE2-CD2	-3.20	118.38	121.95
1	B	111[B]	TOX	CZ2-CE2-CD2	-3.20	118.38	121.95
1	B	111[A]	TOX	CH2-CZ2-CE2	2.63	123.59	118.28
1	B	111[B]	TOX	CH2-CZ2-CE2	2.63	123.59	118.28

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111[A]	TOX	N-CA-CB-CG
1	A	111[A]	TOX	C-CA-CB-CG
1	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	N-CA-CB-CG
1	B	111[A]	TOX	C-CA-CB-CG
1	B	111[B]	TOX	N-CA-CB-CG
1	B	111[B]	TOX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	801	1	50,50,50	1.49	8 (16%)	67,82,82	1.52	12 (17%)
6	PO4	B	805	-	4,4,4	0.85	0	6,6,6	1.17	1 (16%)
2	HEM	B	801	1	50,50,50	1.58	11 (22%)	67,82,82	1.60	11 (16%)
5	OXY	B	804	-	1,1,1	0.11	0	-		
7	MPD	B	806	-	7,7,7	0.97	0	9,10,10	1.73	2 (22%)
6	PO4	A	805	-	4,4,4	0.64	0	6,6,6	1.23	0
7	MPD	A	807	-	7,7,7	0.56	0	9,10,10	1.47	0
7	MPD	A	808	-	7,7,7	0.61	0	9,10,10	1.06	0
7	MPD	A	806	-	7,7,7	0.52	0	9,10,10	1.23	1 (11%)
5	OXY	A	804	-	1,1,1	0.10	0	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	801	1	-	2/14/54/54	-
2	HEM	B	801	1	-	2/14/54/54	-
7	MPD	B	806	-	-	5/5/5/5	-
7	MPD	A	807	-	-	3/5/5/5	-
7	MPD	A	808	-	-	2/5/5/5	-
7	MPD	A	806	-	-	0/5/5/5	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	FE-NB	4.74	2.09	1.94
2	A	801	HEM	FE-NB	4.28	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	FE-NC	3.61	2.07	1.95
2	A	801	HEM	FE-NC	3.35	2.06	1.95
2	B	801	HEM	C4B-NB	-3.20	1.32	1.38
2	B	801	HEM	C1D-C2D	3.18	1.51	1.44
2	A	801	HEM	C4B-NB	-3.17	1.32	1.38
2	B	801	HEM	C1B-NB	-2.85	1.35	1.40
2	B	801	HEM	C3B-C4B	2.71	1.50	1.44
2	B	801	HEM	O1D-CGD	2.65	1.30	1.22
2	A	801	HEM	O1A-CGA	2.38	1.29	1.22
2	B	801	HEM	CHD-C1D	-2.31	1.33	1.39
2	A	801	HEM	C1A-C2A	2.25	1.49	1.44
2	A	801	HEM	C4D-ND	-2.20	1.36	1.40
2	B	801	HEM	C4C-NC	-2.19	1.35	1.39
2	B	801	HEM	FE-NA	2.16	2.02	1.95
2	A	801	HEM	FE-NA	2.12	2.02	1.95
2	A	801	HEM	O1D-CGD	2.11	1.29	1.22
2	B	801	HEM	CMB-C2B	2.07	1.55	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CHC-C4B-NB	4.01	128.74	124.42
2	B	801	HEM	C1B-NB-C4B	3.98	109.92	105.21
2	A	801	HEM	CAA-CBA-CGA	-3.96	103.17	113.67
2	A	801	HEM	C3D-C4D-ND	3.93	114.48	110.17
7	B	806	MPD	CM-C2-C3	3.77	126.47	110.20
2	B	801	HEM	CMD-C2D-C1D	3.69	130.80	125.03
2	A	801	HEM	CMD-C2D-C1D	3.42	130.38	125.03
2	B	801	HEM	CAA-CBA-CGA	-3.31	104.89	113.67
2	A	801	HEM	CMA-C3A-C4A	3.28	130.42	125.42
2	B	801	HEM	C3B-C4B-NB	-3.20	107.17	109.47
2	A	801	HEM	C4D-ND-C1D	-2.89	101.78	105.21
2	B	801	HEM	CBD-CAD-C3D	2.85	120.40	112.53
2	B	801	HEM	O2D-CGD-CBD	2.72	122.60	114.00
2	A	801	HEM	O2D-CGD-CBD	2.71	122.56	114.00
7	B	806	MPD	O2-C2-C3	-2.67	99.28	109.27
2	A	801	HEM	O1D-CGD-CBD	-2.63	114.74	123.09
2	A	801	HEM	CHA-C4D-ND	-2.61	121.14	124.37
2	A	801	HEM	C2D-C1D-ND	2.60	112.90	109.90
2	B	801	HEM	O1A-CGA-CBA	-2.57	114.94	123.09
2	B	801	HEM	C3D-C4D-ND	2.50	112.91	110.17
2	B	801	HEM	O1D-CGD-CBD	-2.41	115.45	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	805	PO4	O4-P-O1	-2.30	102.82	110.95
2	A	801	HEM	C1B-NB-C4B	2.25	107.88	105.21
7	A	806	MPD	O2-C2-C1	-2.18	101.19	107.99
2	B	801	HEM	CAA-C2A-C1A	2.14	129.12	124.94
2	A	801	HEM	CBD-CAD-C3D	2.10	118.34	112.53
2	A	801	HEM	O2A-CGA-CBA	2.06	120.52	114.00

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	807	MPD	C2-C3-C4-C5
7	B	806	MPD	O2-C2-C3-C4
7	B	806	MPD	CM-C2-C3-C4
7	B	806	MPD	C2-C3-C4-C5
7	A	807	MPD	O2-C2-C3-C4
7	A	808	MPD	O2-C2-C3-C4
7	B	806	MPD	C1-C2-C3-C4
7	A	808	MPD	C2-C3-C4-C5
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
7	B	806	MPD	C2-C3-C4-O4
7	A	807	MPD	CM-C2-C3-C4

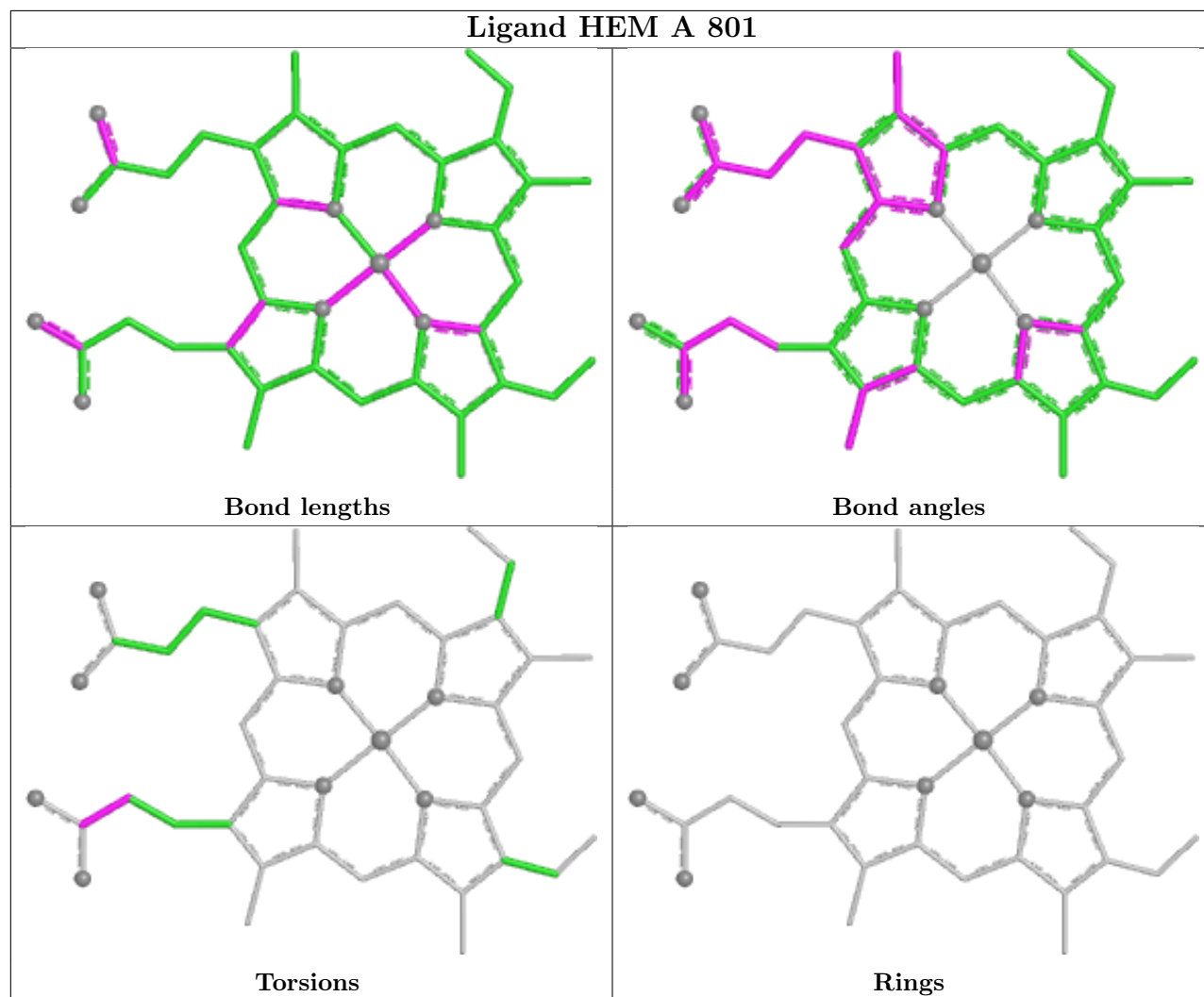
There are no ring outliers.

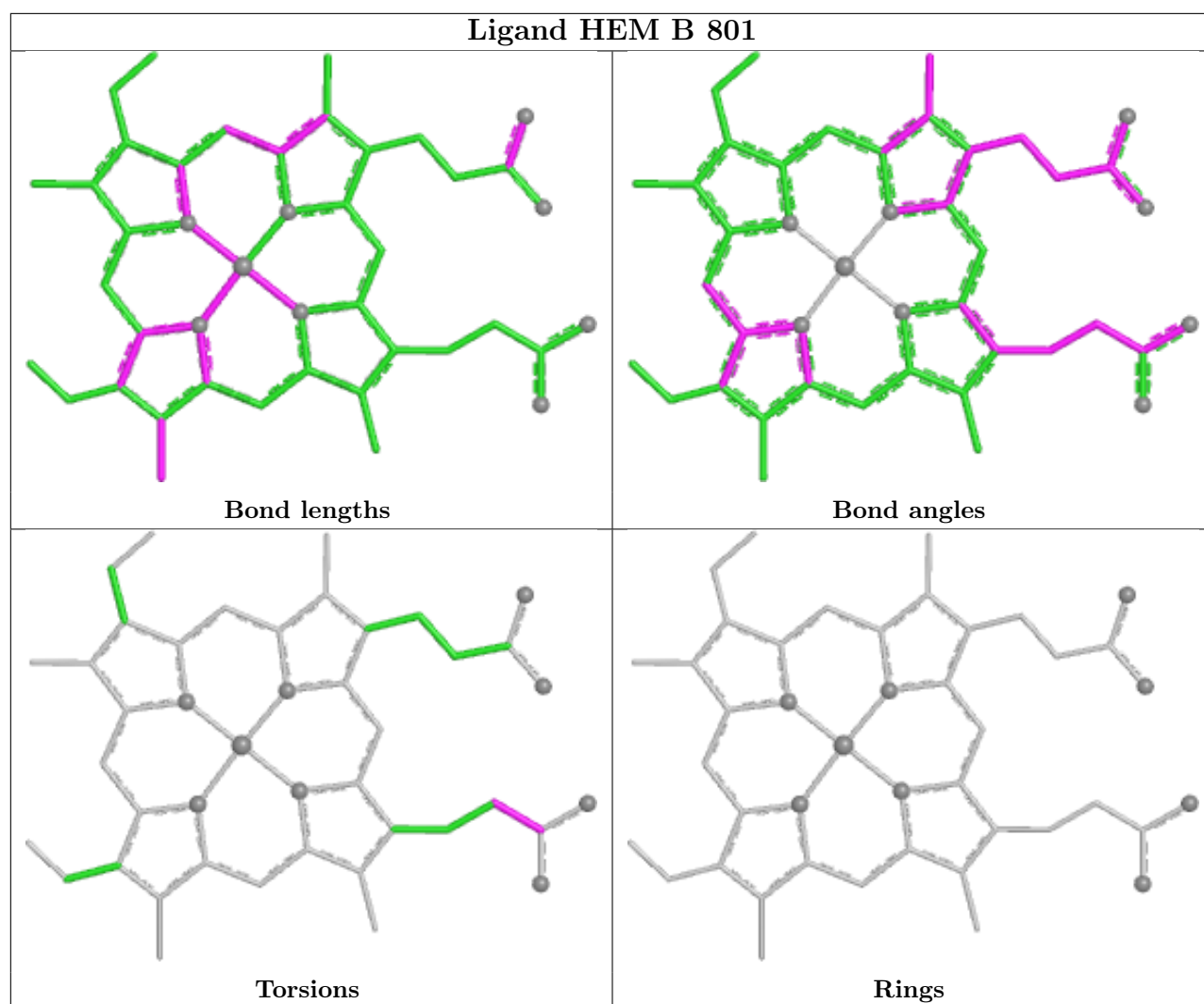
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	806	MPD	1	0
7	A	807	MPD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	712/728 (97%)	-0.19	8 (1%) 78 81	10, 26, 48, 81	6 (0%)
1	B	712/728 (97%)	-0.35	9 (1%) 75 79	9, 25, 44, 81	5 (0%)
All	All	1424/1456 (97%)	-0.27	17 (1%) 76 80	9, 25, 47, 81	11 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	LYS	3.4
1	A	748	ALA	3.2
1	B	679	ALA	2.9
1	A	680	ALA	2.6
1	B	748	ALA	2.6
1	B	682	ALA	2.5
1	B	55	HIS	2.3
1	B	40	ARG	2.3
1	A	119[A]	THR	2.3
1	A	454	ASP	2.2
1	B	65	ASP	2.2
1	A	227	ASN	2.2
1	B	610	ARG	2.2
1	B	680	ALA	2.2
1	B	45	ASN	2.1
1	A	255[A]	ARG	2.0
1	A	215	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TOX	A	111[A]	16/17	0.97	0.06	16,20,23,24	2
1	TOX	A	111[B]	16/17	0.97	0.06	16,20,23,24	2
1	TOX	B	111[A]	16/17	0.98	0.06	16,19,23,24	2
1	TOX	B	111[B]	16/17	0.98	0.06	16,19,22,24	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

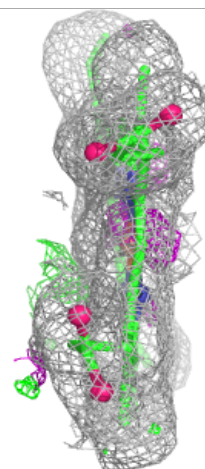
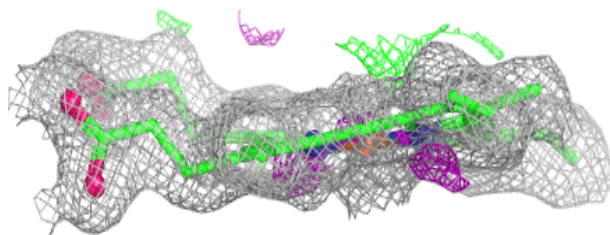
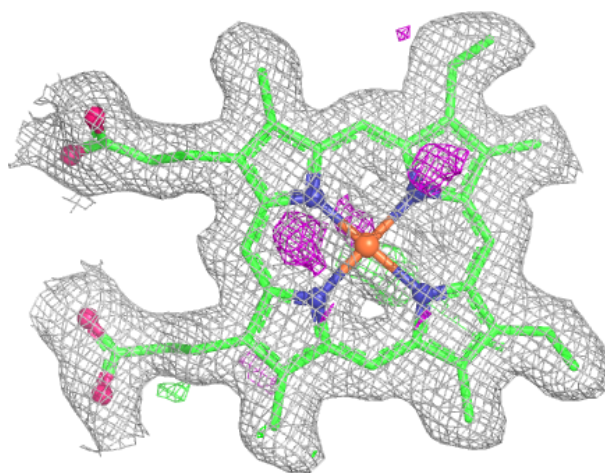
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

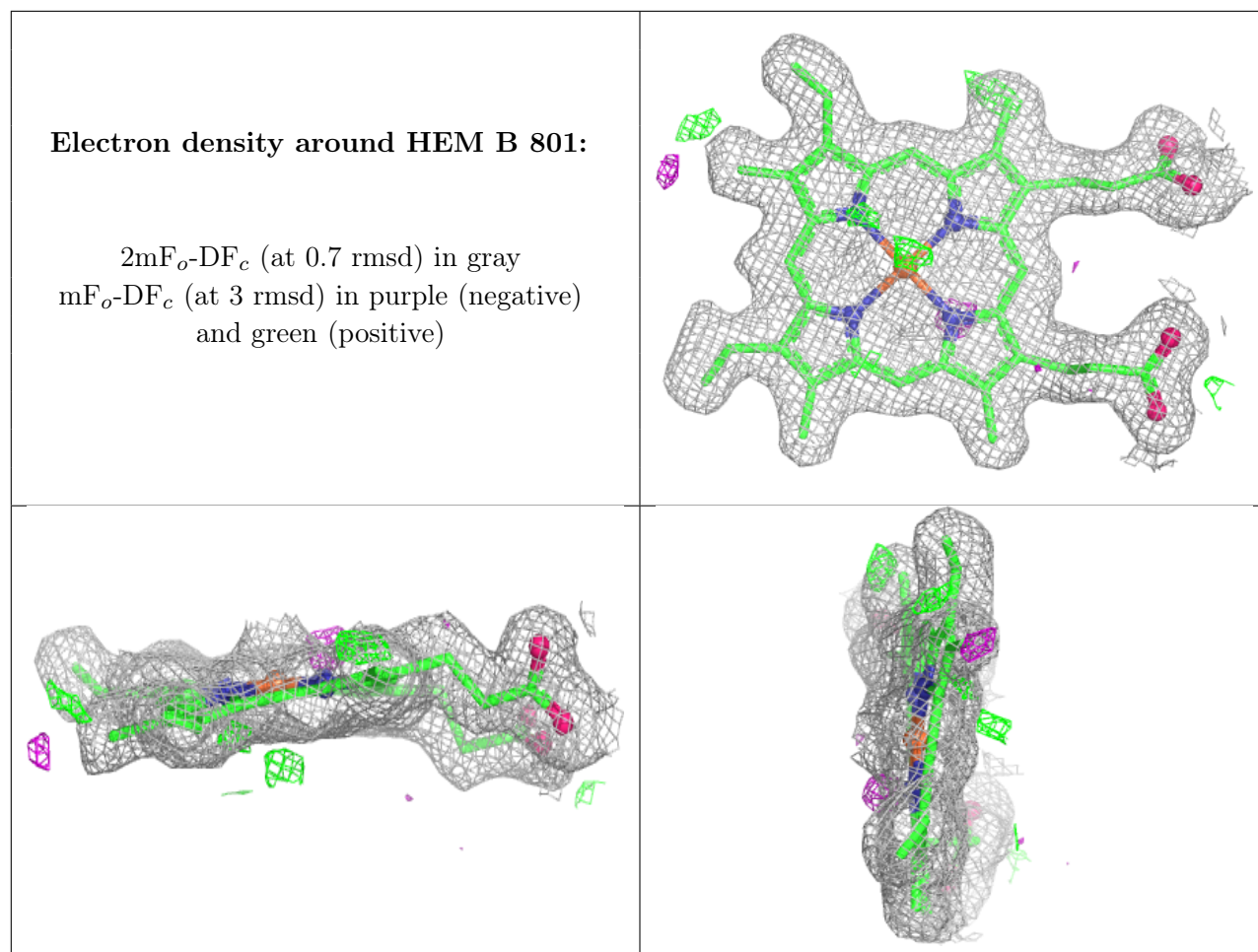
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PO4	A	805	5/5	0.76	0.12	75,76,86,91	0
7	MPD	A	808	8/8	0.86	0.18	72,80,81,90	0
7	MPD	A	806	8/8	0.89	0.20	60,62,72,78	0
5	OXY	A	804	2/2	0.90	0.15	42,42,42,44	0
7	MPD	B	806	8/8	0.91	0.18	48,53,67,75	0
7	MPD	A	807	8/8	0.92	0.14	44,48,51,54	0
5	OXY	B	804	2/2	0.93	0.08	32,32,32,40	0
6	PO4	B	805	5/5	0.93	0.10	49,56,63,64	0
4	CL	A	803	1/1	0.95	0.08	50,50,50,50	0
2	HEM	A	801	43/43	0.98	0.06	18,21,26,28	0
4	CL	B	803	1/1	0.98	0.06	33,33,33,33	1
3	NA	A	802	1/1	0.99	0.07	20,20,20,20	0
3	NA	B	802	1/1	0.99	0.06	21,21,21,21	0
2	HEM	B	801	43/43	0.99	0.05	17,19,21,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.